

Identifiability of Restricted Structural Equation Models

Networks: Processes and Causality, Menorca

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Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich



What is the Problem?

Random variables:

X : water temperature of Mediterranean Sea

Y : # networks and causality related workshops in Cala Galdana

Z : # scientists on Menorca

What is the causal structure?

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- Understand the (physical) process in more detail.

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- Understand the (physical) process in more detail.
- Intervene: Organize workshop in Cala Galdana! Go swimming!

What is the Problem?

Random variables:

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What is the causal structure?

- Understand the (physical) process in more detail.
- Intervene: Organize workshop in Cala Galdana! Go swimming!
- Use observational data!

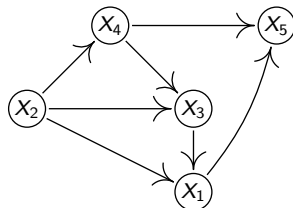
What is the Problem?

observed iid data
from $P(X_1, \dots, X_5)$

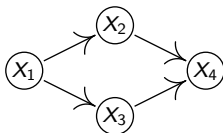
X_1	3.4	1.7	-2.4	...
X_2	-0.2	7.0	-1.2	...
X_3	-0.1	4.3	-0.7	...
X_4	0.3	5.8	0.3	...
X_5	3.5	1.9	-1.9	...



causal DAG \mathcal{G}_0



Relating Causal Graph and Joint Distribution



1 Markov Condition:

$$X_1 \perp\!\!\!\perp X_4 \mid \{X_2, X_3\}$$

$$X_2 \perp\!\!\!\perp X_3 \mid \{X_1\}$$

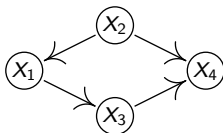
(*d*-separation \Rightarrow cond. independence)

2 Faithfulness:

no more

(no *d*-separation \Rightarrow no cond. independence)

Relating Causal Graph and Joint Distribution



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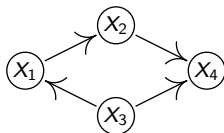
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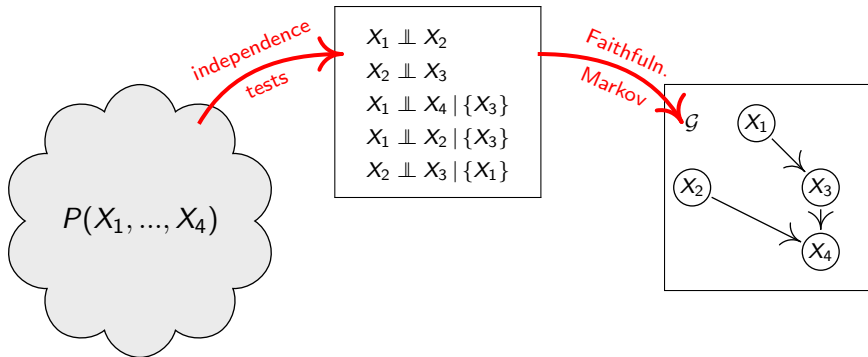
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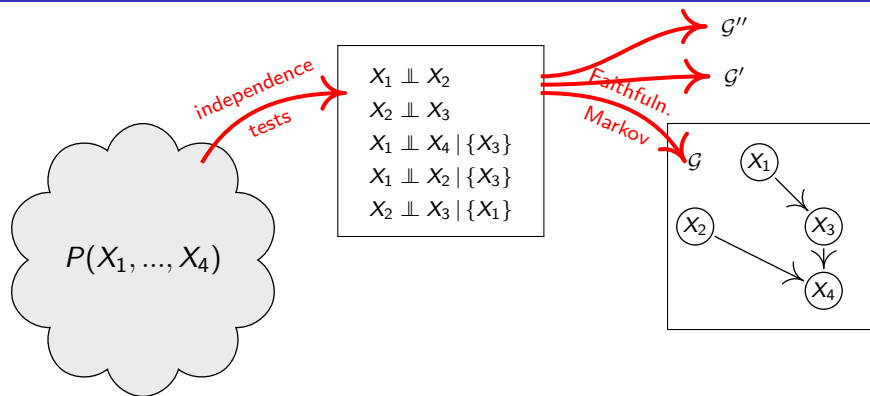
PC Algorithm



Method: PC [Spirtes et al., 2001]

- 1 Find all (cond.) independences from the data.
- 2 Select the DAG(s) that corresponds to these independences.

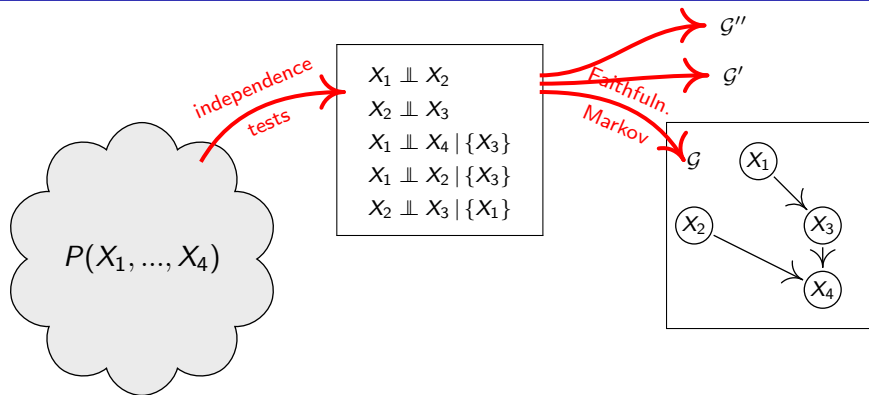
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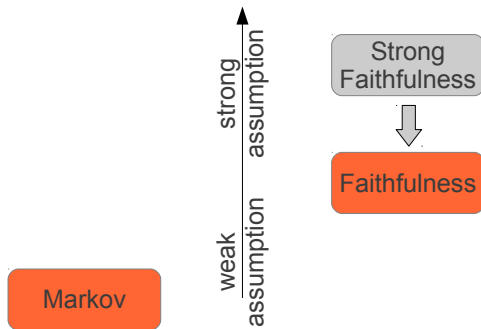
- 1 Find all (cond.) independences from the data. **Be smart.**
- 2 Select the DAG(s) that corresponds to these independences.

The PC algorithm makes very few assumptions.

Can we gain something by making more/different assumptions?

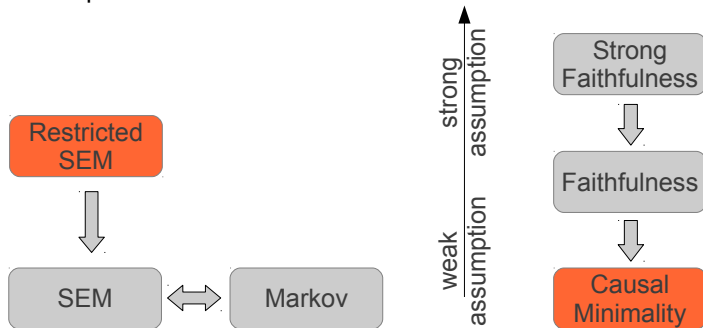
Relating Causal Graph and Joint Distribution

PC assumptions:



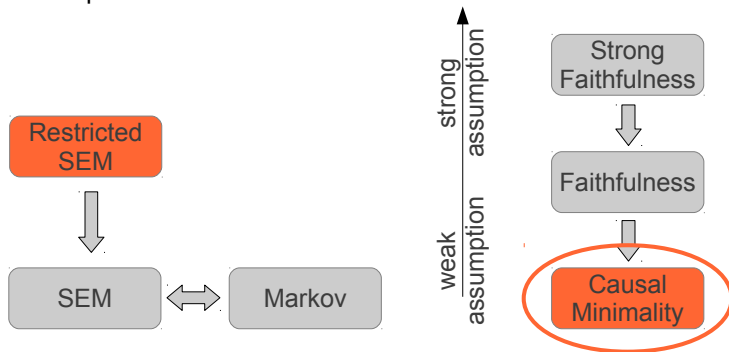
Relating Causal Graph and Joint Distribution

New assumptions:



Relating Causal Graph and Joint Distribution

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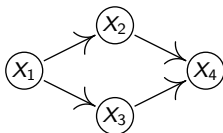
Causal Minimality is a weak form of faithfulness:

Definition

Let \mathcal{G}_0 be the true causal graph. If $P(X_1, \dots, X_p)$ is not Markov to any proper subgraph of \mathcal{G}_0 , causal minimality is satisfied.

\rightsquigarrow “Each arrow does something.”

Violation of Causal Minimality



1 Markov Condition:

$$X_2 \perp\!\!\!\perp X_3 \mid \{X_1\}$$

$$X_1 \perp\!\!\!\perp X_4 \mid \{X_2, X_3\}$$

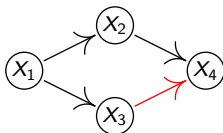
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Violation of Causal Minimality



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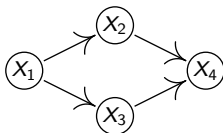
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Violation of Faithfulness



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$$X_1 \perp\!\!\!\perp X_4$$

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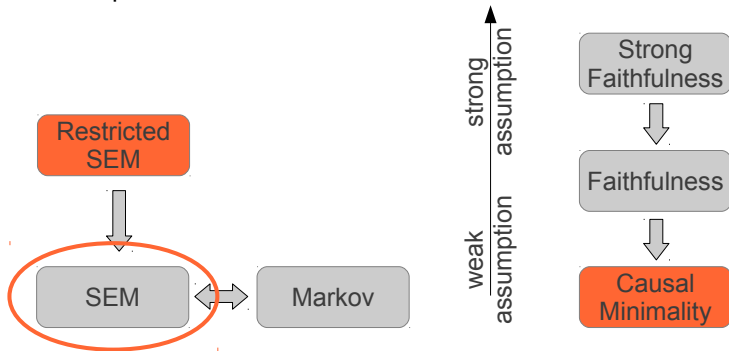
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Relating Causal Graph and Joint Distribution

New assumptions:



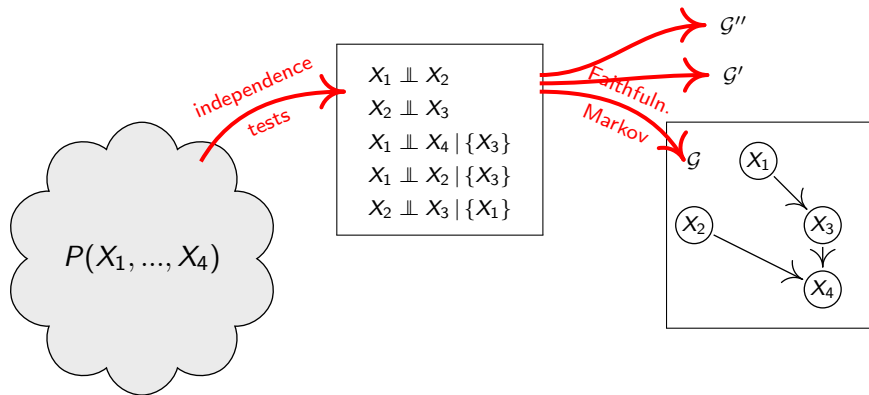
Structural Equation Models

The joint distribution $P(X_1, \dots, X_p)$ satisfies a **Structural Equation Model (SEM)** with graph \mathcal{G}_0 if

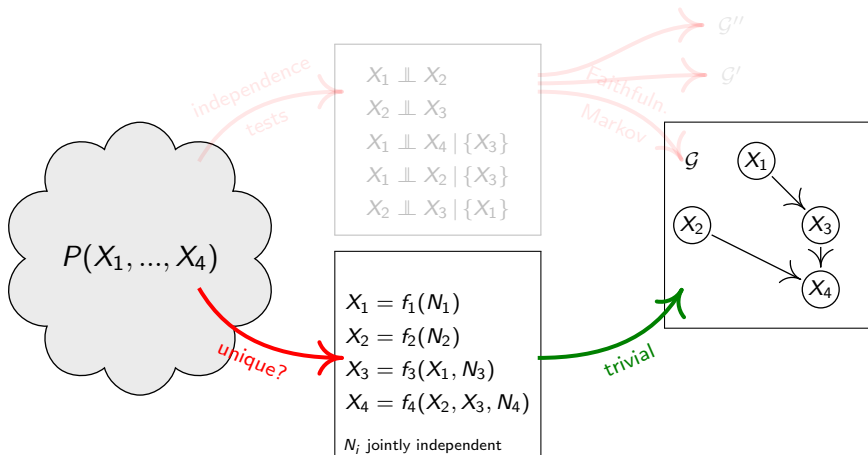
$$X_i = f_i(\mathbf{PA}_i, N_i) \quad 1 \leq i \leq p$$

with \mathbf{PA}_i being the parents of X_i in \mathcal{G}_0 . The N_i are required to be jointly independent.

The Alternative Route

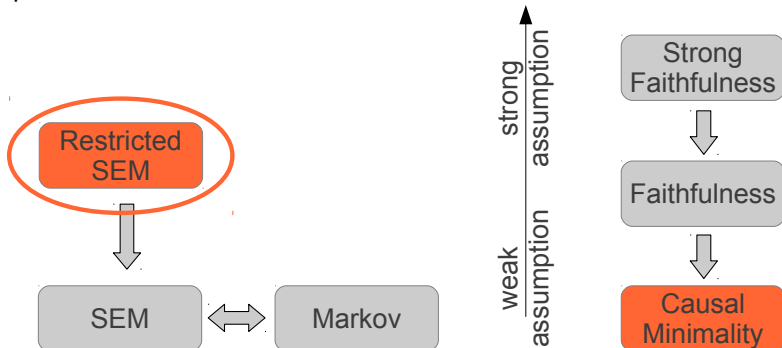


The Alternative Route



Relating Causal Graph and Joint Distribution

New assumptions:



Restricted Structural Equation Models

- Linear Gaussian Additive Noise Models

$$X_i = \sum_{j \in \text{PA}_i} \beta_j X_j + N_i \quad 1 \leq i \leq p$$

with $N_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_i^2)$ and graph \mathcal{G}_0 .

Proposition

Assume faithfulness. Then one can identify the *Markov equivalence class* of \mathcal{G}_0 from $P(X_1, \dots, X_p)$.

Restricted Structural Equation Models

- Linear **Non-Gaussian** Additive Noise Models

$$X_i = \sum_{j \in \text{PA}_i} \beta_j X_j + N_i \quad 1 \leq i \leq p$$

with $N_i \stackrel{\text{iid}}{\sim}$ **non-Gaussian** and graph \mathcal{G}_0 .

(One can show: $\beta_j \neq 0 \Rightarrow$ causal minimality.)

Theorem ([Shimizu et al., 2006])

One can identify \mathcal{G}_0 from $P(X_1, \dots, X_p)$.

Restricted Structural Equation Models

- Linear Gaussian Models with **same Error Variance**

$$X_i = \sum_{j \in \text{PA}_i} \beta_j X_j + N_i \quad 1 \leq i \leq p$$

with $N_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$.

(One can show: $\beta_j \neq 0 \Rightarrow$ causal minimality.)

Theorem ([Peters and Bühlmann, 2012])

One can identify \mathcal{G}_0 from $P(X_1, \dots, X_p)$.

Restricted Structural Equation Models

- **Non-Linear** Additive Noise Models

$$X_i = f_i(X_{\text{PA}_i}) + N_i \quad 1 \leq i \leq p$$

with N_i iid and graph \mathcal{G}_0 .

Theorem ([Hoyer et al., 2009, Peters et al., 2011b])

Exclude a few combinations of f_i and N_i . Then one can identify \mathcal{G}_0 from $P(X_1, \dots, X_p)$.

Restricted Structural Equation Models

- **Discrete** Additive Noise Models

$$X_i = f_i(X_{\text{PA}_i}) + N_i \quad 1 \leq i \leq p$$

with $N_i \stackrel{\text{iid}}{\sim}$ **non-uniform** and graph \mathcal{G}_0 .

Theorem ([Peters et al., 2011a,b])

Exclude a few combinations of f_i and N_i . Then one can identify \mathcal{G}_0 from $P(X_1, \dots, X_p)$.

Restricted Structural Equation Models

Assumption

Assume that $P(X_1, \dots, X_p)$ follows any of the restricted SEMs mentioned above with graph \mathcal{G}_0 and assume causal minimality.

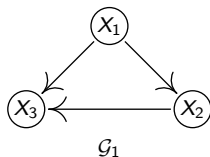
Theorem

Then, the true causal DAG can be recovered from the joint distribution.

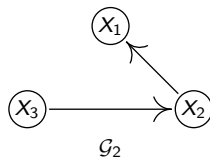
Linear Gaussian Models with fixed Variance

Proof Idea:

Assume $P(X_1, X_2, X_3)$ allows for two SEMs leading to \mathcal{G}_1 and \mathcal{G}_2 :



$$X_3 = \alpha_1 X_1 + \alpha_2 X_2 + N_3$$

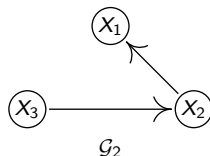
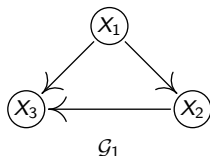


$$X_3 = M_3$$

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$$X_3 = \alpha_1 X_1 + \alpha_2 X_2 + N_3$$

$$X_3^* := X_3|_{X_1=x} = \alpha_1 x + \alpha_2 X_2|_{X_1=x} + N_3$$

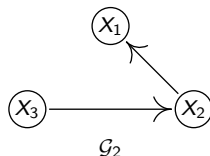
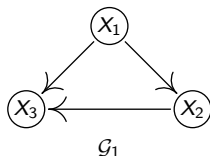
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$$\Rightarrow \text{var}(X_3^*) = 0 + \alpha_2^2 \text{var}(X_2|_{X_1=x}) + \sigma^2 > \sigma^2$$

$$X_3 = M_3$$

$$X_3^* := X_3|_{X_1=x} = M_3|_{X_1=x}$$

$$\Rightarrow \text{var}(X_3^*) \leq \sigma^2$$

Method: IFMOC (Identifiable Functional Model Class)

Idea: If we fit a wrong SEM, noise variables become dependent.

- 1 Find *all* SEMs that fit the data.
- 2 If there is exactly one, output the DAG. Otherwise: “I do not know”.
- 3 Avoid enumerating all DAGs [Mooij et al., 2009]: always find sink and remove additional edges at the end.

needed:

- regression method (e.g. linear, GP),
- independence test (e.g. HSIC).

Method: GDS (Greedy DAG Search)

Only for: linear Gaussian models with same noise variances.

Idea: Define a score (e.g. BIC) to a given DAG.

- 1 Start with random DAG.
- 2 At each step, look at all neighbouring DAGs.
- 3 Go to DAG with best score.

Both:

- + Identifiability within Markov equivalence class.
- + Option to say “I do not know.”
- + No faithfulness.
 - Strong structural assumptions.
 - Not scalable to high-dimensional problems (yet :-)).

Restricted Structural Equation Models

Experiment 1: Comparison IFMOC and PC when both assumptions are met.

sample size: 400
#data sets: 100
 $\alpha = 5\%$



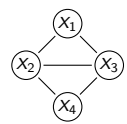




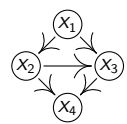


$$X_1 = N_1$$

$$X_2 = N_2$$

$$X_3 = f_3(X_1, X_2) + N_3$$

$$X_4 = f_4(X_2, X_3) + N_4$$

$$N_i \stackrel{\text{iid}}{\sim} \mathcal{U}([-0.5, 0.5]).$$

	linear	nonlinear	
PC _{lin}			
PC _{nonlin}			
IFMOC _{lin}			
IFMOC _{nonlin}			

correct/wrong/no decision

Restricted Structural Equation Models

Experiment 2: How often are we close to non-faithfulness?

#data sets: 500, $\alpha = 5\%$.

$$X_1 = \beta_1 N_1$$

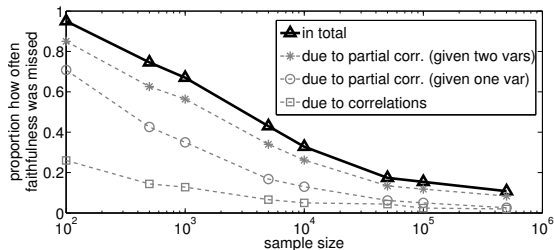
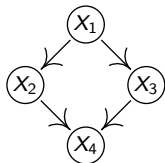
$$X_2 = \gamma_{12} X_1 + \beta_2 N_2$$

$$X_3 = \gamma_{13} X_1 + \beta_3 N_3$$

$$X_4 = \gamma_{24} X_2 + \gamma_{34} X_3 + \beta_4 N_4$$

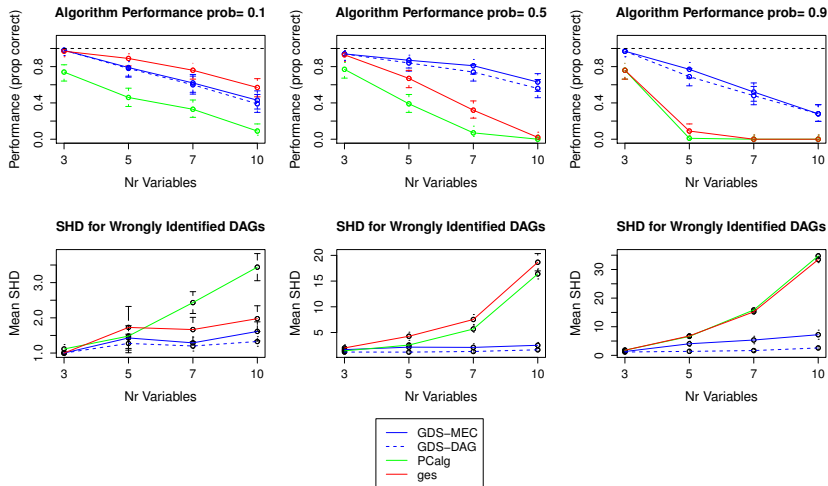
$$N_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1),$$

$$\gamma_{ij} \stackrel{\text{iid}}{\sim} \mathcal{U}([-5, 5]), \beta_i \stackrel{\text{iid}}{\sim} \mathcal{U}([0, 0.5]).$$



Restricted Structural Equation Models

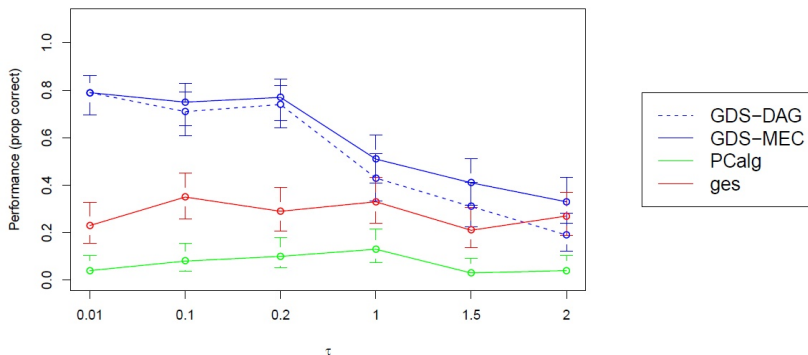
Experiment 3: Linear Gaussian Models with Fixed Variances (GDS).



coefs sampled from $\mathcal{U}([-1.5, -0.1] \cup [0.1, 1.5])$; $n = 1000$; 100 repetitions

Restricted Structural Equation Models

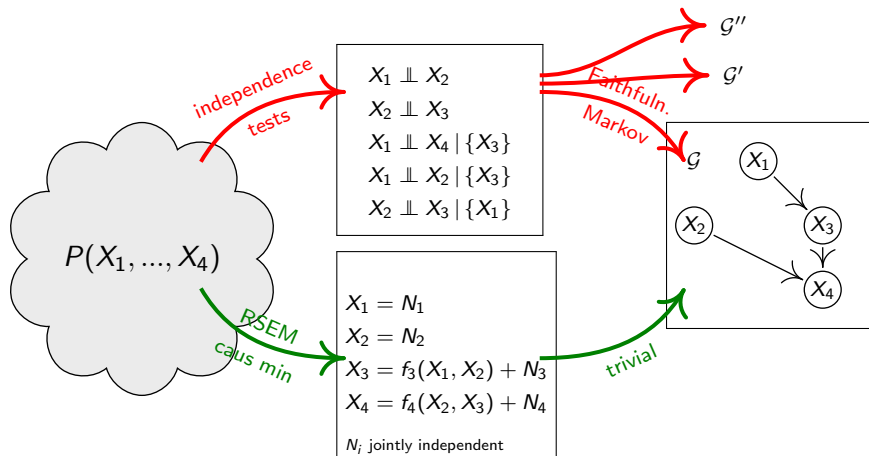
Experiment 4: Violation of Same Error Variances.



noise variances sampled from $\mathcal{U}([4 - \tau, 4 + \tau])$

$n = 1000$, $p = 7$, $prob = 0.5$, 100 repetitions

Summary



¡Muchas gracias!

- P. Hoyer, D. Janzing, J. Mooij, J. Peters, and B. Schölkopf. Nonlinear causal discovery with additive noise models. In *NIPS 21*, 2009.
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- P. Spirtes, C. Glymour, and R. Scheines. *Causation, Prediction, and Search*. MIT Press, 2nd edition, 2001.
- K. Zhang and A. Hyvärinen. On the identifiability of the post-nonlinear causal model. In *UAI 25*, 2009.

Restricted Structural Equation Models

Experiment 1a: Both methods should work when both assumptions are met.

sample size: 400
#data sets: 100
 $\alpha = 5\%$



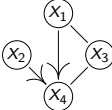




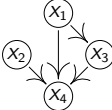


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PC_{lin}			
PC_{nonlin}			
$IFMOC_{\text{lin}}$			
$IFMOC_{\text{nonlin}}$			

correct/wrong/no decision

- Understand relations to Bayesian Network Learning.
- Joint independence of noise \leftrightarrow joint independence noise to ancestors.
- Discrete Confounder.
- Extensive tests on real data, especially on data sets with > 2 variables.
- Robustness.

Markov Condition and Faithfulness

Let \mathcal{G} be the true causal graph of X_1, \dots, X_p .

Assumption (Markov Assumption)

X_i and X_j are *d-separated* by \mathcal{S} in \mathcal{G} \Rightarrow $X_i \perp\!\!\!\perp X_j \mid \mathcal{S}$

Markov Condition and Faithfulness

Let \mathcal{G} be the true causal graph of X_1, \dots, X_p .

Assumption (Markov Assumption)

X_i and X_j are d -separated by S in \mathcal{G} \Rightarrow $X_i \perp\!\!\!\perp X_j \mid S$

Assumption (Faithfulness Assumption)

X_i and X_j are d -separated by S in \mathcal{G} \Leftarrow $X_i \perp\!\!\!\perp X_j \mid S$

Method: IFMOC (two variables)

- 1 Assume an ANM from cause to effect.
- 2 Fit $Y = f(X) + N$ and $X = g(Y) + M$ and check which of the two models lead to independent residuals.
- 3 If only one direction does, output it. Otherwise do not decide.

Independence of Conditional and Marginal

Suppose X is the cause and Y effect. What if

$$Y \neq f(X) + N, \quad N \perp\!\!\!\perp X,$$

but

$$X = g(Y) + M, \quad M \perp\!\!\!\perp Y?$$

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Janzing and Steudel [2010]: This implies “dependence” (based on Kolmogorov complexity) between

$$p(\text{cause}) \text{ and } p(\text{effect} \mid \text{cause})$$

One rather expects input and mechanism to be most often “independent” [Lemeire and Dirkx, 2006, Janzing and Schölkopf, 2010].

Definition (Bivariate Identifiable Set)

We call a set $\mathcal{B} \subseteq \mathcal{F} \times \mathcal{P}_{\mathbb{R}} \times \mathcal{P}_{\mathbb{R}}$ containing combinations of functions $f \in \mathcal{F}$ and distributions $P(X), P(N)$ of input X and noise N *bivariate identifiable in \mathcal{F}* if the following holds:

Identifiable Functional Model Class (IFMOC)

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$$\begin{aligned} & (f, P(X), P(N)) \in \mathcal{B} \quad \text{and} \quad Y = f(X, N), N \perp\!\!\!\perp X \\ \Rightarrow & \quad \exists g \in \mathcal{F} : \quad X = g(Y, M), M \perp\!\!\!\perp Y \end{aligned}$$

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Additionally we require

$$f(X, N) \not\perp\!\!\!\perp X \tag{1}$$

for all $(f, P(X), P(N)) \in \mathcal{B}$ with $N \perp\!\!\!\perp X$.

Identifiable Functional Model Class (IFMOC)

Lemma

The following sets are bivariate identifiable:

(i) linear ANMs [Shimizu et al., 2006]: $\mathcal{F}_1 = \{f(x, n) = ax + n\}$

$$\mathcal{B}_1 = \{(X, N) \text{ not both Gaussian}\} \setminus \tilde{\mathcal{B}}_1$$

(ii) discrete ANMs [Peters et al., 2011b]: $\mathcal{F}_2 = \{f(x, n) \equiv \phi(x) + n(\tilde{m})\}$

$$\mathcal{B}_2 = \{(\phi, X) \text{ not affine and uniform}\} \setminus \tilde{\mathcal{B}}_2$$

(iii) non-linear ANMs [Hoyer et al., 2009]

$$\mathcal{B}_3 = \{(\phi, X, N) \text{ not lin., Gauss, Gauss}\} \setminus \tilde{\mathcal{B}}_3$$

(iv) post-nonlinear ANMs [Zhang and Hyvärinen, 2009]

Identifiable Functional Model Class (IFMOC)

How can we transfer these identifiability results to p variables?

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Definition (\mathcal{F} -FMOC)

- p equations

$$X_i = f_i(\mathbf{PA}_i, N_i) \quad 1 \leq i \leq p$$

are called a *functional model* if N_i are jointly independent and the corresponding graph is acyclic.

Identifiable Functional Model Class (IFMOC)

How can we transfer these identifiability results to p variables?

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- A set of functional models is called a *functional model class with function class \mathcal{F}* , for short *\mathcal{F} -FMOC*, if each of the functional models satisfies $f_i \in \mathcal{F}$ for all i .

Identifiable Functional Model Class (IFMOC)

Definition ((\mathcal{B}, \mathcal{F})-IFMOC)

Let \mathcal{B} be bivariate identifiable in \mathcal{F} . An \mathcal{F} -FMOC is called a (\mathcal{B}, \mathcal{F})-Identifiable Functional Model Class, for short (\mathcal{B}, \mathcal{F})-IFMOC, if for all its functional models

$$X_i = f_i(\mathbf{PA}_i, N_i), \quad 1 \leq i \leq p$$

and for all $1 \leq i \leq p$, $j \in \mathbf{PA}_i$, for all sets $\mathbf{S} \subseteq \{1, \dots, p\}$ with $\mathbf{PA}_i \setminus \{j\} \subseteq \mathbf{S} \subseteq \mathbf{ND}_i \setminus \{i, j\}$ we have:

There exists an $x_{\mathbf{S}}$ with $p_{\mathbf{S}}(x_{\mathbf{S}}) > 0$ and

$$\left(f_i(x_{\mathbf{PA}_i \setminus \{j\}}, \underbrace{\cdot}_{X_j}, \underbrace{\cdot}_{N_i}), P(X_j | X_{\mathbf{S}} = x_{\mathbf{S}}), P(N_i) \right) \in \mathcal{B}. \quad (2)$$

Identifiable Functional Model Class (IFMOC)

Experiment 1b: Both methods should work when both assumptions are met.

sample size: 400
#data sets: 100
 $\alpha = 5\%$



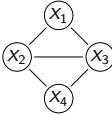






$$X_1 = f_1(N_1)$$

$$X_2 = f_2(N_2)$$

$$X_3 = f_3(X_1, X_2, N_3)$$

$$X_4 = f_4(X_2, X_3, N_4)$$

$N_i \stackrel{\text{iid}}{\sim} \mathcal{U}([-0.5, 0.5]).$

	linear	nonlinear	
$PC_{\text{part.corr}}$			
PC_{HSIC}			
$IFMOC_{\text{lin}}$			
$IFMOC_{\text{GP}}$			

correct/wrong/no decision

Restricted Structural Equation Models

Experiment 2: If the distribution is not faithful, PC fails, IFMOC does not.

sample size: 1000

#data sets: 100

$\alpha = 5\%$


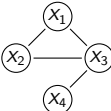

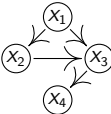
$$X_1 = N_1$$

$$X_2 = 1.5X_1 + N_2$$

$$X_3 = 3X_1 - 2X_2 + N_3$$

$$X_4 = 1.8X_3 + N_4$$

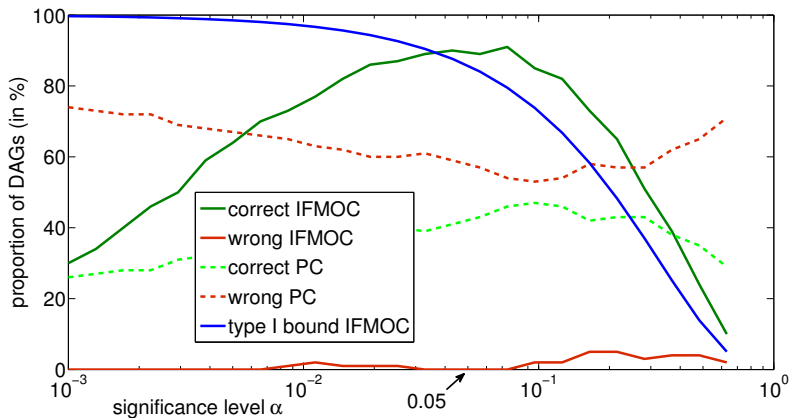
with $N_i \stackrel{\text{iid}}{\sim} \mathcal{U}([0, 0.5])$.

	linear	
PC_{lin}		
$IFMOC_{\text{lin}}$		

correct/wrong/no decision

Identifiable Functional Model Class (IFMOC)

Experiment 2b: Both methods should work when both assumptions are met.



Identifiable Functional Model Class (IFMOC)

already known: 2 variable case

Theorem (Hoyer et al. [2009])

Let

$$Y = f(X) + N, \quad N \perp\!\!\!\perp X.$$

Then for most combinations $(f, P(X), P(N))$

$$X \neq g(Y) + M, \quad M \perp\!\!\!\perp Y.$$

Those combinations $(f, P(X), P(N))$ are called *bivariate identifying*.

Identifiable Functional Model Class (IFMOC)

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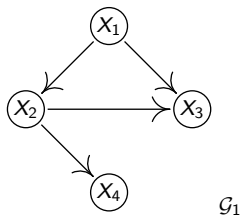
Similar results for

- (i) post-nonlinear additive noise [Zhang et al., 2009]
- (ii) discrete additive noise [Peters et al., 2011b]

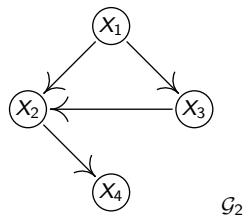
What happens in the case of p variables?

Identifiable Functional Model Class (IFMOC)

Assume $P(X_1, X_2, X_3, X_4)$ allows for two functional models leading to \mathcal{G}_1 and \mathcal{G}_2 :



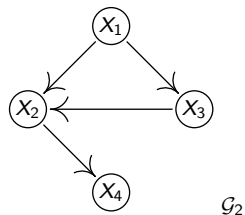
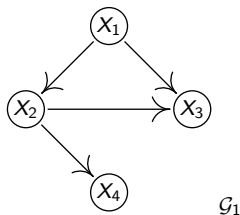
$$X_3 = f(X_1, X_2, N_3)$$



$$X_2 = g(X_1, X_3, N_2)$$

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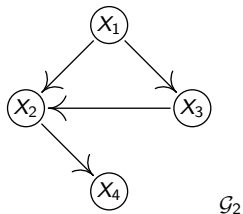
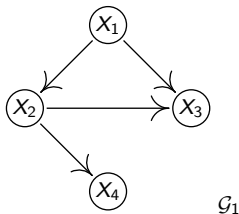
$$X_3 = f(X_1, X_2, N_3)$$

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$$\Rightarrow X_3|_{X_1=x} = f(x, X_2|_{X_1=x}, N_3)$$

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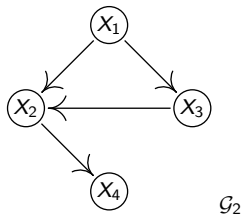
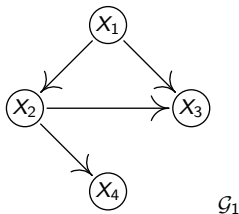
$$X_3 = f(X_1, X_2, N_3)$$

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$$\Rightarrow \begin{aligned} X_3|_{X_1=x} &= f(x, X_2|_{X_1=x}, N_3) \\ X_2|_{X_1=x} &= g(x, X_3|_{X_1=x}, N_2) \end{aligned}$$

Identifiable Functional Model Class (IFMOC)

Assume $P(X_1, X_2, X_3, X_4)$ allows for two functional models leading to \mathcal{G}_1 and \mathcal{G}_2 :



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If the triple $(f(x, \cdot, \cdot), P(X_2|_{X_1=x}), P(N_3))$ is bivariate identifying, then \checkmark .

Identifiable Functional Model Class (IFMOC)

Definition (IFMOC)

- A set of functional models is called a *functional model class with function class \mathcal{F}* , for short \mathcal{F} -FMOC, if each of the functional models satisfies $f_i \in \mathcal{F}$ for all i .
- An \mathcal{F} -FMOC is called an *Identifiable Functional Model Class*, for short IFMOC, if for all its functional models

$$X_i = f_i(\mathbf{PA}_i, N_i), \quad 1 \leq i \leq p$$

and for all $1 \leq i \leq p$, $j \in \mathbf{PA}_i$, for all sets $\mathbf{S} \subseteq \{1, \dots, p\}$, $\mathbf{S} \cap \{i\} = \emptyset$, $\mathbf{S} \cup \{i\} \subseteq \mathbf{S} \subseteq \mathbf{ND}_i \setminus \{i, j\}$ there exists an $x_{\mathbf{S}}$ with $p_{\mathbf{S}}(x_{\mathbf{S}}) > 0$ and

based on bivariate identifiability

$$\left(\underbrace{f_i}_{X_j}, \underbrace{f_i}_{N_j}, P(X_j | X_{\mathbf{S}} = x_{\mathbf{S}}), P(N_j) \right) \text{ is bivariate identifying.} \quad (3)$$